

Structural Materials Under Extreme Conditions

A MaRIE Workshop
Los Alamos National Laboratory, July 29-31, 2009

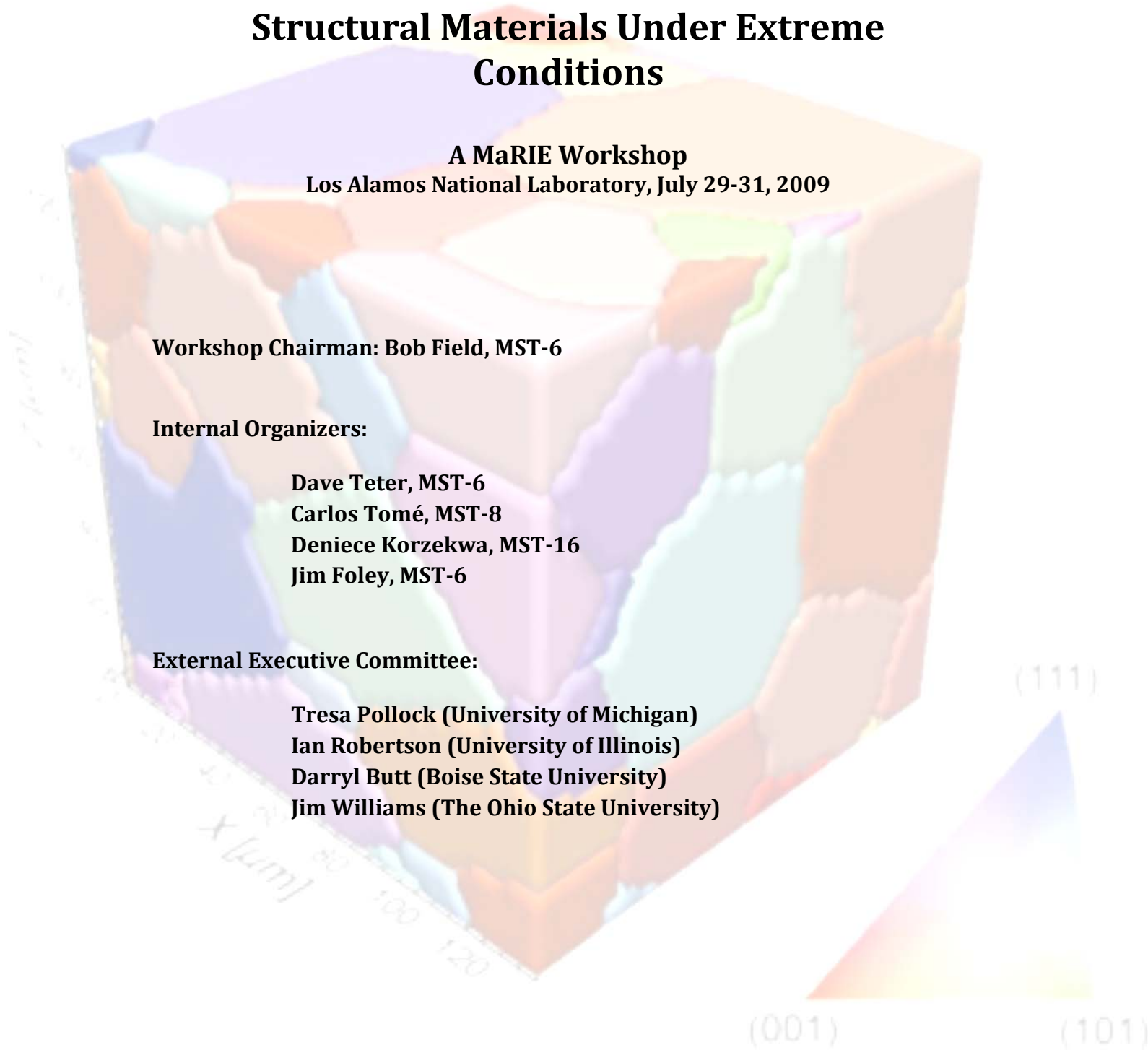
Workshop Chairman: Bob Field, MST-6

Internal Organizers:

Dave Teter, MST-6
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External Executive Committee:

Tresa Pollock (University of Michigan)
Ian Robertson (University of Illinois)
Darryl Butt (Boise State University)
Jim Williams (The Ohio State University)



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LANL Internal Organizers

Materials Needs—Specific Applications—Chair: Dave Teter

Materials Modeling—Chair: Carlos Tome

Materials Processing—Chair: Deniece Korzekwa

Characterization—Chair: Bob Field

Specific Properties/Materials Interactions—Chair: Jim Foley

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Executive Summary of MaRIE Workshop on Structural Materials

LANL is in the process of holding a series of focused workshops designed to engage the external scientific community and help define the facilities and capabilities to be incorporated into MaRIE. A three-day workshop focused on structural materials was held July 29-31, 2009 at LANL. The purpose of the workshop was to assess future needs in structural materials applications and supporting research, and to identify the developments and innovation necessary in the next ~10 years. Of particular interest was the development of in situ characterization techniques during processing, synthesis, and functioning of structural materials, along with supporting modeling to develop a predictive capability of materials performance.

The workshop was structured around a series of talks by both internal and external experts in structural materials development, production, application, and characterization. Speakers and attendees represented industry, academia and other National Laboratories. The talks and group discussions were asked to build upon current state-of-the-art work to define the experimental and modeling capabilities that will not only shape of the future of materials research at LANL and more broadly, but provide a new set of tools for the structural materials community at large. An external executive committee composed of Tresa Pollock (U. Michigan), Ian Robertson (U. Illinois), Darryl Butt (Boise State U), and Jim Williams (Ohio State U) played an important role in defining the overall structure of the workshop and the conclusions that emerged.

The workshop was organized into five sessions: (1) materials needs – specific applications, (2) materials modeling, (3), materials processing (4) materials characterization, and (5) specific properties/materials interactions. At the end of the talks we brought the speakers back to the front of the auditorium to facilitate a broader discussion based upon what was presented during the session and previous sessions. Recommendations were made in the following areas:

Common Scientific Needs

- Pressing technical problems
- Integrated Computational Materials Engineering (ICME)
- Broad range of environments for in situ experiments
- Multiscale capability
- Wide range of spatial and temporal resolution
- Multiple probes/detectors for simultaneous recording of disparate data
- New detector technology optimized for Materials Science
- 3D analysis
- Data management and analysis
- Data archiving and sharing

User Facility Considerations

- Flexible/modular design
- Shared experimental tools
- User support
- Educational component
- Hazardous/difficult materials
- Ancillary characterization facilities
- Computational capability

MaRIE Specific Technical Recommendations

- An integrated modeling/experimental approach is vital to the future of materials development. The approach for MaRIE in this area should be consistent with ICME.
- Multiple in situ extreme environments are needed to simulate real life conditions as closely as possible and investigate complex mechanisms of materials degradation and failure. This will require a flexible facility that can accommodate complex experimental apparatus.
- Major breakthroughs in the understanding of fundamental materials phenomena will require simultaneously active multiple probes and detectors to fully characterize the specimen during in situ experiments.
- Coordinated multiscale modeling and experiments are critical to success. The latter will require multiple probes with a range of spatial and temporal resolution and real time analysis of data in order to zero in on “hot spots” in the microstructure for more detailed analysis.
- In addition to the advanced probes proposed for MaRIE, advanced detector development could have significant impact on the community at relatively low cost.
- Advanced n-D microstructural characterization techniques and the tools to analyze the enormous data sets are needed. (n is 3D for spatial, plus time, grain orientation, strain, chemical signature, etc).
- There is a need for a large-scale facility dedicated to environmental/corrosion science. MaRIE could fulfill this need.
- There is a need for a facility that can routinely handle radioactive/hazardous material, with the ability to store samples for further analysis. MaRIE could fulfill this need.
- There is a need for a large-scale facility for in situ characterization of materials during processing (e.g. casting, thermomechanical processing, welding, etc.). MaRIE could fulfill this need.
- State-of-the-art characterization and modeling tools are needed in addition to the “beamline tool” for a more enhanced experience for visiting users. Example: having SEM, TEM, FIB, atom probe, spectroscopy available to further characterize the sample ex situ, with transfer capability between in situ experimental site and ancillary capabilities.
- MaRIE should have a strong educational component to develop personnel for interdisciplinary teams needed for the future success of this type of facility.

- Shared experimental tools, data, and models would strongly enhance the impact of a user facility. A NIH model could be implemented. NIH requires that models and data be available to all who are funded by NIH. “Superusers” with enhanced funding/access would have a greater opportunity/responsibility for developing sharable tools.
- Customer support in setting up experiments, and acquiring, storing, and processing huge amounts of information is vital for the user. General software and hardware should be maintained by the facility, with personnel allocated to this function.
- Effective data archiving and open dissemination is central to the future of collaborative materials research. This must be developed upfront at a high level, not in an ad hoc manner by individual researcher/groups.
- The mission of MaRIE should focus on only 2-3 major materials challenges and address them comprehensively and holistically. MaRIE would develop personnel, tools and integrated models that solve complex problems and lead to new materials solutions.

A1. Workshop Summary - Introduction

LANL is in the process of holding a series of focused workshops designed to engage the external scientific community and help define the facilities and capabilities to be incorporated into MaRIE. A three-day workshop focused on structural materials was held July 29-31, 2009 at LANL. The purpose of the workshop was to assess future needs in structural materials applications and supporting research, and to identify the developments and innovation necessary in the next ~10 years. Of particular interest was the development of in situ characterization techniques during processing, synthesis, and functioning of structural materials, along with supporting modeling to develop a predictive capability of materials performance.

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A2. Workshop Summary – Session/Presentation Summaries

Materials Needs - Specific Applications (Weds. 7/29 –AM) – Chair: Dave Teter

Integrated Computational Materials Engineering (ICME): A New and Essential Capability for Surviving Extreme Environments in the Automotive Industry, John Allison (Ford Motor Company)

This presentation outlined the challenges facing the auto industry, specifically Ford Motor Company. Dr. Allison presented the ICME concept promoted by the National Academy of Engineering (NAE) (see Figure 1) and an application of the ICME framework to the specific problem of Al alloy castings. The industry is driving materials design to provide faster turnaround, higher quality, lower costs, smaller and lighter components, and improved fuel economy and performance, all in an industry that has had to cut costs 50% in a year! Specific materials challenges noted

were (1) lightweight materials (AHSS, Al, Mg, CFRP); (2) high temperature and high strength materials for advanced power trains, and increased exhaust temperatures – primarily for improved fuel efficiency; (3) electrification (HEV/Plug-in/Full Electric): battery materials and manufacturing technology for zero fossil fuel use.

Ford implemented the ICME approach to casting modeling using a combination of continuum (OPTCAST), thermodynamic (ThermoCalc) and empirical (PanDat and Dictra) modeling in a serialized approach. Empirical models are costly, requiring significant amounts of materials testing to develop an accurate model, and cannot easily be extrapolated to other material systems or conditions. An opportunity exists in the area of microstructural modeling, currently not well implemented in the design models. Ford is exploring phase field modeling to develop accurate predictions of precipitate kinetics for modeling microstructural evolution.

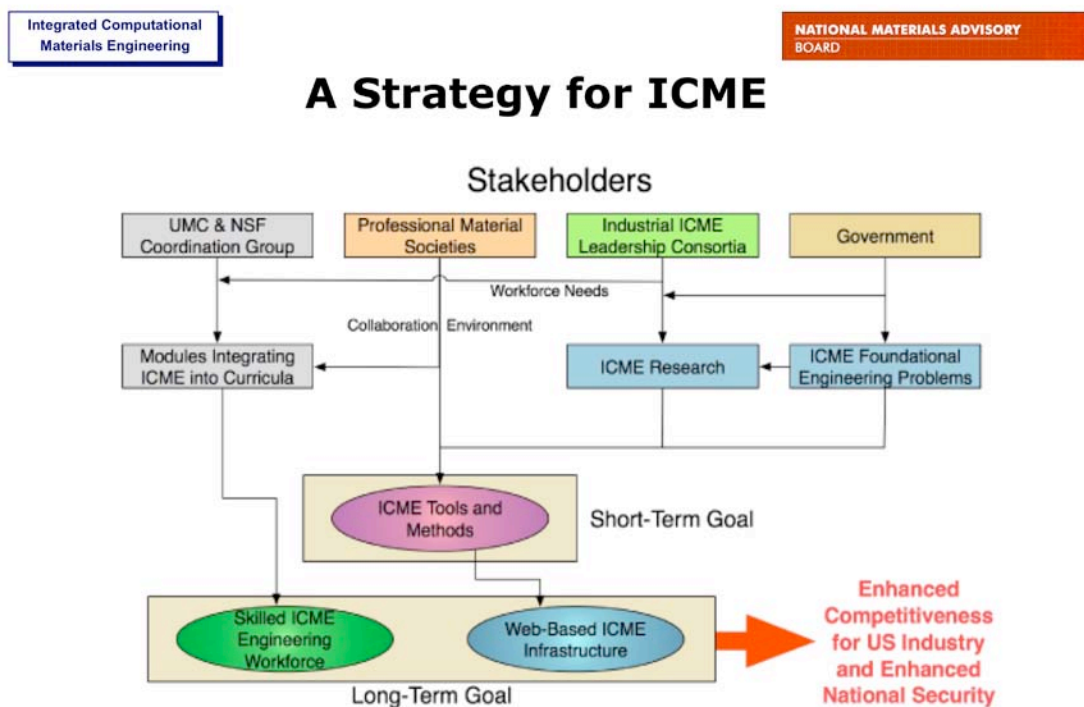


Figure 1. Integrated Computational Materials Engineering (ICME) strategy (J. Allison)

Structural Challenges in Nuclear Energy Systems, Steve Zinkle (Oak Ridge National Laboratory)

For advanced nuclear reactor designs and extension of current reactor lifetimes, a number of technological challenges must be addressed, including dose-temperature windows and burn-up limits, enhanced safety, minimized waste streams, and proliferation resistance. In the development of advanced materials for nuclear

reactor application, the economic impact must also be considered. Depending on the type of improvement, the net capital cost may be less or significantly greater than the current material design.

One of the goals of the nuclear energy industry is to have zero fuel failures by 2010, which requires being able to predict fuel life so maintenance can be planned. In order to achieve the goal of 100% failure-free performance, we need to address a wide range of physical mechanisms causing failure, including cladding-material corrosion, hydrogen content in cladding, oxide spallation (local blisters), radiation damage, and cracking. Radiation damage can cause large changes to structural materials, limiting their lifetimes. Phenomena which require a more quantitative understanding are: (1) radiation hardening and embrittlement ($<0.4 T_M$, >0.1 dpa), (2) phase instabilities from radiation-induced precipitation ($0.3-0.6 T_M$, >10 dpa), (3) irradiation creep ($<0.45 T_M$, >10 dpa), (4) volumetric swelling from void formation ($0.3-0.6 T_M$, >10 dpa), and high temperature He embrittlement ($>0.5 T_M$, >10 dpa).

Gen III and IV reactors require new materials with higher operating temperatures ($>300^\circ\text{C}$) and radiation damage limits ($>50\text{dpa}$). Thermodynamic and kinetic tools will be required to develop new alloys. Advanced characterization tools for highly radioactive materials are also needed; current facilities do not allow this, although some user facilities are becoming more open to the examination of radioactive samples.

Aerospace Materials, Jim Williams (The Ohio State University)

Materials problems in jet engines, rocket engines, and hypersonic aircraft were discussed in this presentation. The speaker stressed the importance of being able to develop new materials using a combined experimental/modeling approach to predict properties/performance in real applications, with a variety of environmental factors, including temperature, stress, pressure, time of exposure, rate of change of any of these, constant or cyclic exposure, and physical environments (e.g. air, vacuum, corrosive, H_2 gas, radiation). Large changes in any of these compared to previous experience represent an “extreme”. Interpolation is possible if functional dependence is known, but extrapolation is risky. The difficulty is to accurately represent actual environments during experiments and properly define input parameters and interactions in modeling.

Major issues in jet engines are maximum operating temperature and time at temperature in hot sections. Rocket engines are more limited by large transients and gradients as well as H_2 and O_2 exposure. Hypersonic vehicles face extreme temperatures, requiring thermal protection, and ultraviolet exposure. Ni-base superalloys are currently operating at 80% of melting temperature, approaching their limits. Future advances are likely to come from hybrid materials (e.g. multi-materials systems with adaptive microstructures: MMSAM) with locally tailored properties. These can be made up of multiple classes of materials (e.g. metals/ceramics/polymers) or single classes with variations in composition and/or microstructure. These hybrid systems present new challenges in development and

property/performance prediction. Lastly, the speaker emphasized that materials are generally limited by minimum rather than average properties, so that understanding the weakest link in a microstructure is often most important (e.g. in fatigue). This concept was explored further in Prof. Jones' presentation on fatigue.

Materials Challenges in Oil and Gas Industry, Greg Kusinski and Jim Skogsberg (Chevron)

The two speakers addressed the two primary areas of concern for the industry: upstream (production, i.e. wells) and downstream (refining) processes. Similar issues arise in both cases, mostly revolving around corrosion/environmental properties. The vast scale of materials required also introduces large economic factors, pushing selection criteria in the direction of less expensive materials. Mechanistic understanding of degradation/failure mechanisms can go a long way to improving performance, lowering costs, increasing lifetimes (or inspection intervals), improving safety, and reducing environmental impact.

Corrosion environments vary widely, with concerns about chlorides (HCl), sulfur (H₂S), amines, high molecular weight carboxylic acids, naphthenic acid, and hydrogen effects at various temperatures (100-500°C), with other complications including high fluid flows (erosion), high pressures, and thermal shock. Carbon steels are preferred for cost reasons, but Cr-Mo steels, stainless steels, and Ni-base alloys are also used. The ability to go to lower cost materials is highly desirable (e.g. higher strength/corrosion resistant low alloy steels or development of stainless steels to replace Ni-base alloys). There is a critical need for new materials or use of existing materials in new applications (e.g. Ti alloys or composites). The main interest with respect to facilities like MaRIE is the development of realistic in situ corrosion testing and modeling to predict performance of these materials. This requires proper definition of the environments (a significant challenge in itself, as pointed out by Prof. Williams) and testing under multiple, simultaneous environmental conditions, with multiple probes to assess complex mechanisms.

Group Discussion

Much of the discussion revolved around the role of modeling and supporting experimental work on reducing development time and cost and increasing the useful life of components by more accurately predicting failure. A systems (holistic) approach to modeling was advocated, along the lines of ICME. This would include integrated models of processing, performance, and failure, taking into account materials variability with the introduction of probabilistic distributions of defects. Experiments must more closely mirror actual application environments, so that critical failure mechanisms are not missed. This requires test cells to accommodate multiple environmental factors (e.g. temperature, stress/pressure, corrosive media, radiation, etc.) as well as multiple probes to evaluate material response.

The goal is not necessarily to eliminate the need for component/certification testing, but to better define the failure modes with increased confidence so that fewer, more targeted tests can be performed. Similarly, more robust models can be coupled with in-service diagnostics and NDE inspections to better predict failure, allowing

extended service of deployed components. This goal requires an integrated modeling approach, which does not necessarily capture all of the physics, but provides performance windows that can be used to drive development and guide in-service evaluation and repair/retirement decisions.

Materials Modeling (Weds. 7/29 -PM) – Chair: Carlos Tome

“Modeling and Experimental Characterization of Local Features (stress, strain, microstructure)”, Carlos Tome (Los Alamos National Laboratory)

“Interrogating Grain Scale Deformation within a Polycrystalline Alloy using New Micromechanical Testing Techniques and Crystal-Based Elastic Plastic Material Models”, Matthew Miller and Paul Dawson (Cornell University)

The presentations by Tomé and Miller tackled modeling of polycrystal aggregates and identified structural features relevant to the models and measurable using diffraction techniques. Both presenters have experience with neutron and X-ray synchrotron diffraction techniques. Both emphasized the need for 3D characterization of grain structures (morphology and orientation), plus capabilities for distinguishing size and shape of voids, twins or cracks. Both emphasized the need for measuring local strains as a conduit for calculating local stresses: resolution of local plastic effects at grain boundaries, near voids and twins, and intragranular stress-strain gradients. Typically 10 μ m features should be resolved for comparison to models. Depending on deformation regime (creep, quasi-static, high rate) full in-situ measurements of stress-strain evolution should be performed either instantly (as snapshots) and/or without interrupting deformation (in a continuous manner). In any case, full structure characterization times of the order of seconds are desired.

Numerically efficient mesoscopic models based on homogeneous deformation of grains embedded in an effective medium can be validated using Finite Element (FE) or Fast Fourier Transform (FFT) methods, which solve stress equilibrium and calculate local stresses and strains. Diffraction experiments will be used, in turn, to validate the FE or FFT results. At this scale, experiments and models co-validate, since neither is exactly assured. It is desired to measure hundreds of grains and to characterize their full stress tensors. Alternatively, it is also desired to focus on specific regions, such as in the vicinity of voids, cracks, twins, or grain boundaries, and measure localization effects in detail (~100nm). Once validated, the local numerical characterization will be used to benchmark Effective Field and Phase Field models, which are faster but based on homogenization assumptions.

“Multiscale Modeling of Deformation in Metals Under Extreme Conditions”, Hussein Zbib (University of Washington)

“Phase Field Modeling of Coupled Displacive-Diffusional Processes”, Yunzhi Wang (The Ohio State University)

The presentations by Zbib and Wang were more concerned with microscopic scales of materials. Dislocation cores, defect-dislocation interactions, irradiation cascade

dynamics and defect production, micro-cracking, transmissibility of dislocation across interfaces, radiation strengthening, nanolayer strength, mobility of dislocations, diffusivity, and precipitation.

Their models rely on Molecular Dynamics (MD) approaches coupled to Dislocation Dynamics (DD) or Phase Field methods (see Figure 2). The advantage of this approach is that very specific microscopic deformation mechanisms can be unraveled, especially at high rates, where experimental characterization is difficult. The spatial scale of the calculations is of the order nm's and time scale in μ s's. The presentations focused well on modeling issues but did not necessarily address the connection with potential experimental characterization. The characterization of dislocations and cascades will require in-situ TEM and 3D characterization capabilities.

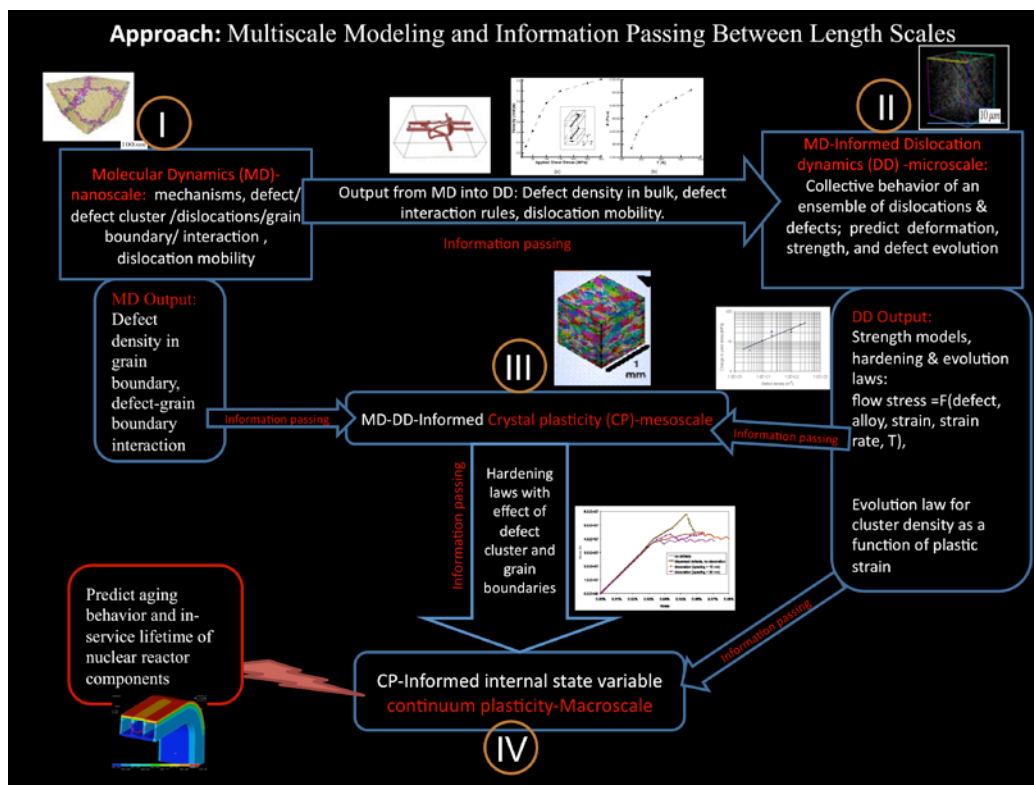


Figure 2. Multiscale plasticity modeling approach (H. Zbib)

Group Discussion:

Much of the discussion dealt with the experimental data needed to validate the models. The need for subgrain (100nm) resolution as well as sufficient temporal resolution to yield time resolved data without stress relaxation during the measurement was stressed. More details about dislocation core structure, intragrain dislocation structures, and transmission across boundaries are needed.

The subject of how to deal with stochastic processes was also discussed. Most models are deterministic, but material response exhibits a good deal of local variability. Phase field methods are well poised for dealing with complex

heterogeneities. Local variability sometimes determines the mechanical outcome. Capturing such variability with models and with experiments is high in the ‘wish list’ of materials scientists. New experimental and modeling approaches may be required for capturing the variability. An ‘ensemble statistics’ approach could be used, modeling several similar systems, taking averages, and comparing with experiments.

Materials Processing (Thurs. 7/30 A) – Chair: Deniece Korzekwa

“Solidification Modeling and Experiments – What we think we know and what we need”, Deniece Korzekwa (Los Alamos National Laboratory)

Solidification modeling is a valuable tool and saves a tremendous amount of time and money over a “trial and error” method of casting. The desire is for casting modeling to be more predictive, but to date the models still rely on a large amount of empirical data. There is a need for better understanding of underlying physics and kinetics as well as more precise data about interfaces and boundary conditions. Two examples of these needs are the undercooling and nucleation observed during phase change and the heat transfer coefficient between the metal and the mold wall (see Figure 3). There is also a need for more physical properties of alloys as a function of temperature, multi-component phase diagrams (equilibrium and metastable), and in situ observation of solidification processes. 3-D information is required to probe the intricacies of the solidification microstructure (see example in Prof. Pollock’s presentation).

Temperature comparisons: simulation and experiment

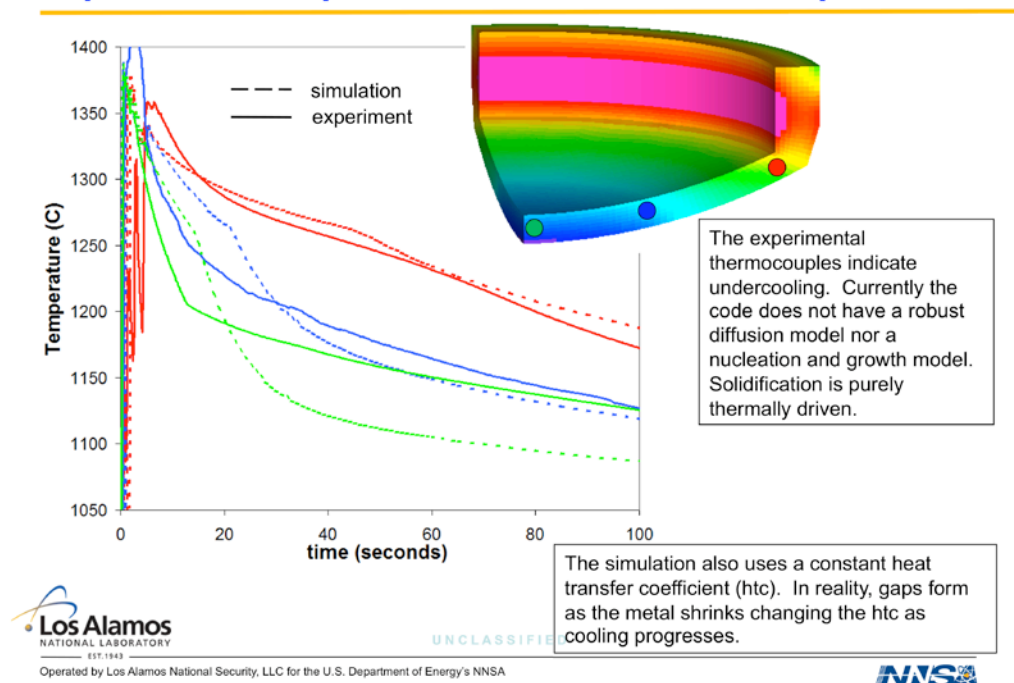


Figure 3. Comparison between casting model and experimental data (D. Korzekwa)

“Role of Joining Science in Developing Hybrid Structural Materials”, Suresh Babu (The Ohio State University)

Joining is even more important as we move to hybrid materials. Prof. Babu posed three challenges: 1) fundamental understanding of joint formation, 2) mapping characterization into material models, and 3) optimization using integrated materials joining models. He also identified three needs: 1) more researchers to address materials joining problems, 2) infrastructure to measure thermo-mechanical transients at good spatial and temporal resolution, and 3) the industrial need for quick answers for rapid deployment with minimum experimentation.

How can we join materials without destroying the microstructure and properties? This is the scientific challenge. Extreme conditions are inherent to fusion processes, especially welding. The process is fast and variable. Thermal-physical material properties during rapid processing conditions are needed. Although integrated models are available to predict the performance of joints, a trial and error approach is still required to develop the correct properties and parameters. The mechanisms involved such high strain rates and high temperature gradients are not well understood. Traditional characterization methods such as EBSD can evaluate only the original and final materials. Thus, there is a need for in situ evaluation with high spatial and temporal resolution.

“Radiation Effects on Metal/Oxide Interfaces”, Darryl Butt (Boise State University)

In nuclear power plants, water/metal interfacial corrosion plays a large part in the lifetime of the reactor. The ability to predict the service and maintenance requirements of all parts within the reactor will significantly reduce costs and failures. Radiolysis plays a large part at the corrosion interface. If the short-lived products at the surface react, we need to understand how the surface oxide and the underlying metal are affected. In most cases the interface structure is not well understood. Future needs include in situ probes to measure the corrosion reactions at the interfaces in radiation environments, remote diagnostics, electrochemical measurements, and multi-scale modeling, particularly of the radiation-corrosion-oxide-metal interface. The importance of education, outreach, long term commitment, collaboration, and collegiality was stressed.

“Exploiting the Power of Powder Synthesis Reactions for Advanced Structural Materials”, Iver Anderson (Ames Laboratory)

Nuclear and coal power plants require a high temperature (900°C), long lifetime, structural material. Oxide dispersion strengthened steels are one option that is being explored. The current processing pathway requires high energy, longtime ball milling for mechanical alloying and results in a product that is prone to contamination and hard to control. Gas atomization followed by hot isostatic pressing (HIP) would be a simplified process, but the atomization needs better characterization and control. The Gas Atomization Reaction Synthesis (GARS) process being developed uses controlled atmospheres during atomization to introduce oxide layers that can diffuse and react during HIP to form dispersoids.

However, the atomization/reaction process is not well understood. We need to understand the wave breakup and droplet formation and be able to image the surface of the droplets and the droplet temperatures. This requires in situ experimental capabilities for imaging two-phase flow with high spatial (10 μ m) and temporal (μ s) resolution. In situ monitoring of oxygen diffusion and dispersoid formation during HIP is also needed. This needs to be coupled with modeling, with phase field modeling approaches of particular interest.

Group Discussion:

Much of the discussion concerned the nature of collaborative research, particularly with respect to large user facilities, and the mission of a facility like MaRIE. There was a consensus on the need for collaboration, as no single institution has the resources to address large technical problems. The consortium approach was discussed, with the Advanced Steel Processing & Products Research Center (ASPPRC) at Colorado School of Mines as an example. One challenge of this approach is handling intellectual property, particularly when specific technology is involved. It was suggested that a CRADA like model might be applicable. A specific question arose as to whether the atomization unit at LANL could be used in conjunction with MaRIE, as research capabilities in this technology are waning.

There was discussion as to the goals of MaRIE and many believed that it should be focused on one - or a few - large problems that can be taken from start to finish (e.g. processing to performance). This was thought to be good both for development and student education and training, but requires processing/production as well as characterization capabilities. MaRIE could be a showcase for this approach. Integration of modeling with experiment was again emphasized, with the need for computing facilities as well as programs on method development and data reduction. The topic of staging and experimental set up was discussed. This is time consuming and the need for assistance in this area was expressed. A modular design with separate staging/set up areas may address this issue.

Characterization (Thurs. 7/30 PM) – Chair: Bob Field

“In Situ Neutron Diffraction Techniques”, Sven Vogel (Los Alamos National Laboratory)

The speaker presented an outline of LANSCE current capabilities, particularly SMARTS and HIPPO. He also summarized proposed and ongoing capability enhancements, including those that are part of the Enhanced Lujan Project. Improvements include a hot cell diffractometer, the LAPTRON instrument (diffraction, radiography, ultrasonic testing, deformation, and calorimetry in a single instrument), as well as improvements in detectors (to increase acceptance angles and time resolution as well as allow for smaller specimens), better beam focusing and collimation, and more user-friendly software to make advanced analysis techniques faster and more routine.

“Characterization of Phase Transformations in Structural Materials Under Extreme” Conditions”, Mike Kaufman (Colorado School of Mines)

The talk emphasized the importance of combining multiple techniques in characterizing microstructures. Specific examples were provided in the use of high resolution (aberration corrected) S/TEM, focused ion beam (FIB), local electrode atom probe (LEAP), and modeling to solve problems of phase transformations, interfaces, and radiation damage. In-situ techniques were also discussed, particularly with regard to S/TEM, including dynamic TEM (DTEM), which has the potential to probe reactions in materials with high temporal and spatial resolution. The speaker also referred to the 2006 NSF Workshop Report: “Dynamic in-situ electron microscopy as a tool to meet the challenges of the nanoworld”, which emphasized the need for centralized facilities and expertise with remote access and teaching capabilities and funding for development of new techniques.

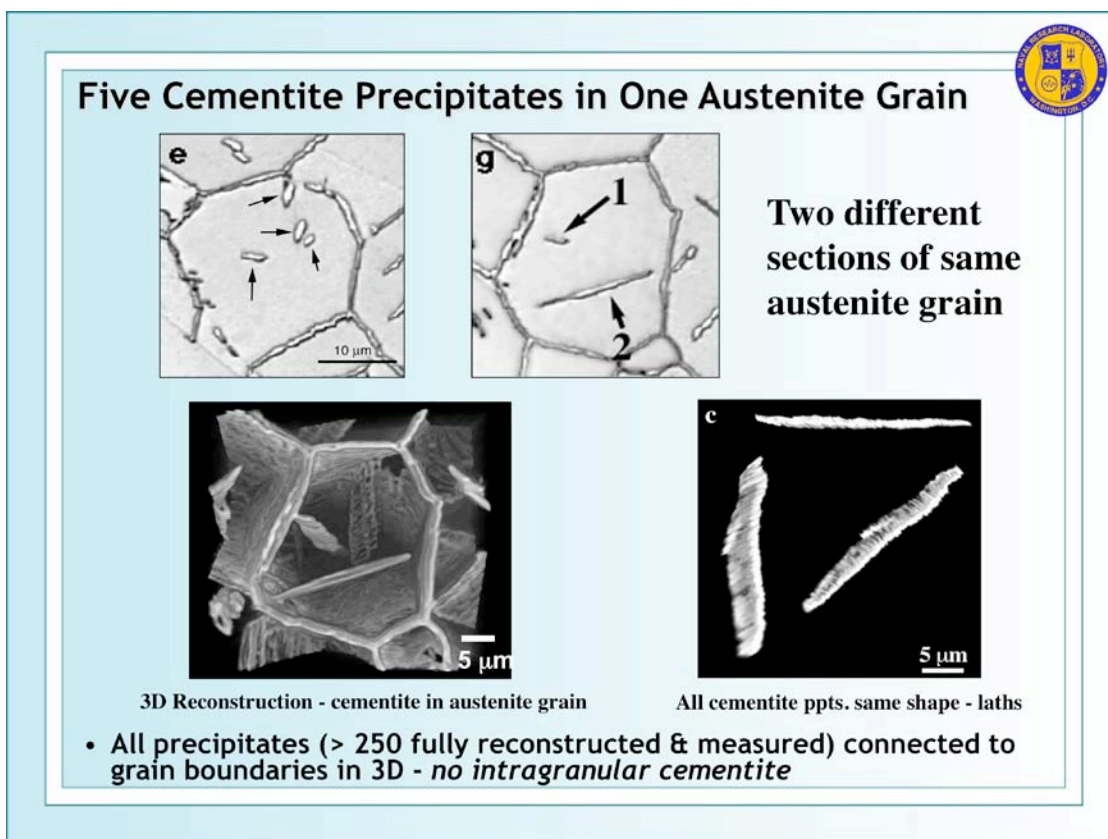


Figure 4. Example of the need for 3-D microstructural characterization techniques (A. Geltmacher: M. V. Kral and G. Spanos, *Acta Materialia*, **47**, 711-724 (1999))

“3D Microstructural Characterization and Analysis”, Andy Geltmacher (Naval Research Laboratory)

A summary was presented of recent work at NRL in 3D data collection, analysis, and modeling. The need for 3D investigations of microstructures was emphasized with examples from real systems in which important aspects of the microstructure are missed in 2D characterization, e.g. “intragranular” cementite in steels is actually all

connected to the grain boundaries, generally to edges and corners (see Figure 4). Also 2D characterization tends to miss “outliers” (e.g. large grains) that can dictate properties. 3D also allows new types of data (e.g. crystallographic interface normal distribution – CINT) to be correlated with properties. Experiment/modeling links were also discussed, including incorporating experimental data into models and more efficient modeling through generating relevant volume elements (RVE) via multiple statistical volume elements (SVE) to generate representative properties. Future needs include higher resolution and larger volume characterization, both in situ and ex situ, better experimental/modeling approaches to achieve “materials by design” goals, and determining microstructure/property relationships from large data sets.

“High Energy X-Ray Diffraction Microscopy: Access to Volumetric Microstructural Responses”, Robert Suter (Carnegie-Mellon University)

The talk summarized high energy x-ray diffraction microscopy (HEDM) techniques, near field measurements (e.g. grain mapping) and far field measurements (e.g. single grain strain distributions). Current spatial resolution is in the micron range for volumes of several mm³; however, collection times are long (~12hrs.). This work generates large data sets; data sets will grow even larger if more details of the microstructure are analyzed, such as strain distributions in association with subgrain boundaries. These techniques can also be combined with microtomography (e.g. to map voids), but association of these features with the microstructure is problematic. Other future challenges include decreased collection times to allow better in situ experiments. This will require small, high flux, high energy beams; fast, efficient, large detectors; and human resources to develop hardware and software to analyze large data sets.

“In-Situ 3D X-Ray Techniques”, Erick Lauridsen (RISO, Denmark)

This talk also involved 3D x-ray techniques, but addressed several different techniques, including several tomography techniques (absorption, phase contrast, diffraction contrast, holo-, and topo-tomography). The speaker emphasized the concept of 4D characterization (3 spatial dimensions and time) and the trade-off between spatial and temporal resolution. Several examples were presented in which simultaneous collection of data using a combination of techniques was used to address different problems. The need for better detectors to improve spatial and temporal resolution was stressed - today’s detectors were developed for the medical imaging industry and are not optimized for materials science problems. The need for high beam quality (flux, brilliance, and stability), simultaneous use of multiple image modalities, and dedicated software development, with special focus on automation and user friendliness to handle large data sets, was also discussed. The need for data analysis was again stressed, as well as archiving. This must be addressed by the experts (many exist in the biological community).

Group Discussion:

The use of multiple, simultaneous characterization techniques is the best approach to solve complex scientific and technical problems, both during an in situ

experiment and before/after. The need for ex situ pre and post experiment characterization was discussed (this is part of the function of the M4 facility). There was a lively discussion of the need for better detectors and better definition of what detectors we need. This is a particularly challenging problem with a multiple probe facility, requiring multiple detectors. We must define what detectors are needed and develop them. Most of the detector technology comes from the medical imaging community and is not optimized for material science. Detector development would be a relatively inexpensive effort (compared to building large beam lines).

Data analysis and archiving at MaRIE will be critical to its success. This includes memory issues (these experiments create huge data files, e.g. in the terabyte range), data reduction, analysis and visualization, and the ability to archive and make widely available large amounts of data. This needs to be done by experts, not ad hoc by individual researchers or groups. The biological community is very good at this and is looking for other areas to apply their tools (Marc DeGraef at Carnegie-Mellon Univ. was given as an example of someone interacting with the biological community in this area). NIH also has requirements for open source of data generated by their funding that promotes collaborative research. The nature of multiscale experiments, vis-à-vis multiscale modeling was also discussed. Modelers start at the fine scale and work up to meso- and macro-scale. Experimenters often do this in reverse, looking at the overall system and then zeroing in on “hot spots”. This requires real time data analysis to recognize areas of interest and focus in on them.

Specific Properties/Materials Interactions (Fri. 7/31 AM)– Chair: Jim Foley

“Challenges in Materials Degradation by Corrosion: Needs for Prognosis and Computational Materials Design”, John R. Scully (University of Virginia)

Prof. Scully pointed out that most corrosion work is empirical with little predictive capability. Moreover, there is a need for a centralized location for corrosion work. This was cast into experimental/modeling approach of ICME (see John Allison’s presentation), with the goal of not only predicting performance of new parts, but residual lifetimes based on inspection. Other needs are the ability to measure isolated electrochemical properties at finer length scales. The multiscale nature of corrosion problems was stressed in this context (see Figure 5). Similar to fatigue, corrosion failure is often driven by defects and local events (weakest element) as opposed to average behavior, making multiscale approaches even more important. Corrosion has some overlap with hydrogen embrittlement, because of the formation of hydrogen during the formation of some corrosion products.

Needs for a facility like MaRIE are: multiple simultaneous tools and probes to advance characterization of governing heterogeneities at sub-micrometer scale (electrochemical, chemical, mechanical, other); ability and create model analogs that can be tested with confidence, exploiting rescaling as necessary (both isolated and reassembled to model complex microstructures); development of models that can accept as inputs environmental stresses, physical, as well as metallurgical factors

and can output properties or attributes, some at the engineering level; and rational connection of length and times scales such that atomic scale information is of value to engineers.

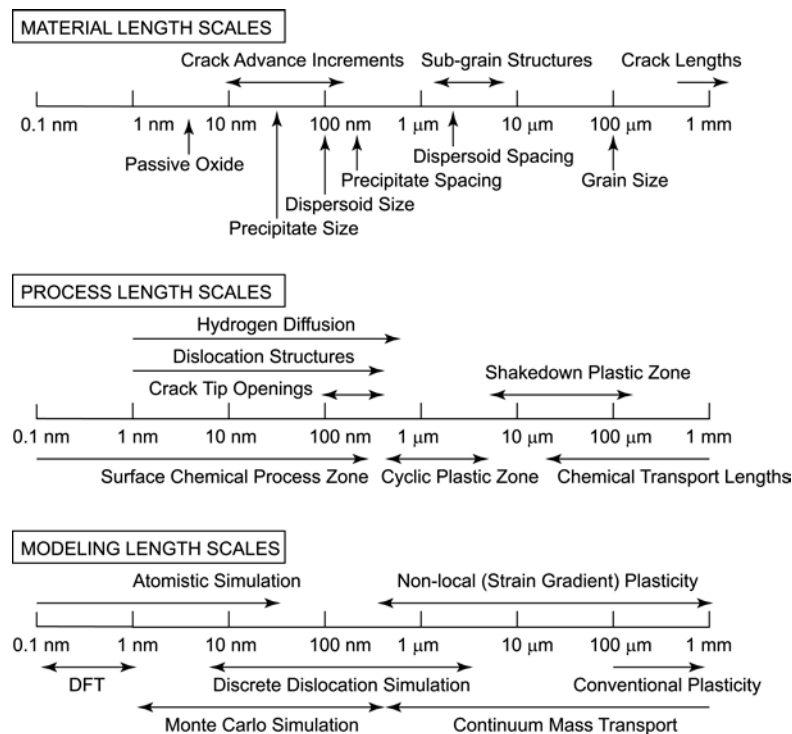


Figure 5. Length scales of corrosion processes and current modeling capabilities (J.R. Scully)

"Hydrogen Embrittlement – current status and future directions", Ian M. Robertson (University of Illinois)

There are several different mechanisms for hydrogen embrittlement; the principal mechanisms are decohesion (either of the general lattice or at defects such as grain boundaries and precipitates) and enhanced plasticity (especially near crack tips) as hydrogen segregates to dislocations. To distinguish between these and determine details of the mechanisms requires us to determine not only how hydrogen gets into a sample, but where the hydrogen is located in a given sample and how it moves. Hydrogen location has to be determined in 3D, dynamically and at the atomic level, in order to have the greatest impact on fundamental understanding.

In situ electron optical techniques have contributed greatly to our understanding of this phenomenon, but higher spatial and temporal resolution techniques will be needed. Hydrogen often acts in concert with other impurities and defects to cause embrittlement. Hydrogen embrittlement has some overlap with fatigue since fatigue resistance is reduced with the presence of hydrogen. Hydrogen embrittlement arises in a number of technological areas, as reflected in other presentations, and therefore represents a challenging problem with broad impact.

“Understanding the Role of Microstructure Variability on Fatigue Behavior”, J. Wayne Jones (University of Michigan)

Prof. Jones presented results from research on very high cycle fatigue (VHCF, $>10^7$ cycles), where the variability of life is so large that the concept of a “fatigue limit” becomes unreliable. In this regime, microstructural variability becomes even more important and the need for multiscale/multiprobe experiments becomes critical. There is a need to identify the weakest volume element (WVE), rather than the representative volume element in modeling as well as experiments. This volume element is no longer necessarily a defect, but a microstructural feature, such as a large grain (or cluster of like oriented grains), carbide, or precipitate/dispersoid cluster. Experimentally, it may be necessary to identify this defect during the experiment and then focus in on it for more detailed analysis. He described in situ experiments conducted at APS to identify initiation sites and follow crack propagation.

In addition to his technical discussion, Prof. Jones commented on the philosophy of a large user center. He stated that such a facility should look for impact, not necessarily uniqueness. He also stressed the importance of building a user infrastructure that supports young faculty members to develop strong collaborations with lab scientists/engineers and other users.

“High Temperature Materials: What Next?”, Tresa Pollock (University of Michigan)

Prof. Pollock pointed out that most extreme engineering systems are limited by the materials from which they are made. She stressed the need for an integrated suite of material models to design materials for multiple conditions, with models driving experimental work. Integration is often more important than complexity, with simple models, representing 80% of the physics, often sufficient if they are integrated to provide a useful design tool. Prof. Pollock presented many examples where an integrated model, based on the ICME approach, could be used to predict the best solution, including turbine discs and hybrid materials solutions for hypersonic vehicles. She stressed the need for 3D analysis, from the μm to cm range, to properly characterize microstructure, with examples of solidification structures using optical techniques and precipitate distributions in steel using a femtosecond laser ablation technique. Prof. Pollock also reiterated the important role of hybrid materials in addressing future materials challenges, with examples including thermal barrier coatings and zero expansion composite structures, consisting of geometrical arrangements of diverse materials that minimized differential expansion effects.

Prof. Pollock’s thoughts on user facilities reflected her belief (widely held by the participants) that the future of materials research rests on large, collaborative projects requiring archival databases and models to promote interdisciplinary collaboration. She pointed to success stories from other communities, such as the genome project, in which specific, quantitative goals and a structure that promoted collaboration and data dissemination contributed to the success. This included “Support of research training of pre and postdoctoral fellows until a critical mass of

students with the right combination of computational and experimental skills is available”.

Group Discussion:

Most of the discussion concerned how the facility should be set up and operated. The consensus was that the community is too fragmented and MaRIE could be a model for promoting open, collaborative research. This should include not only collaborators connected by funding (the traditional approach) but by a common scientific problem. The vision was a large collaborative team, both on and off site, working on any given experiment, requiring remote as well as local facility access. Remote access for experimenters would also be useful for training and preparation for experiments, maximizing the use of on-site time.

The importance of educational out reach was also emphasized. The need for local assistance for setting up experiments was discussed: from things as simple as having a machine shop for last minute modifications or repairs, to instrument specialists to assist users, ex situ characterization capabilities, and computational capabilities (hardware and software) – not just a “here’s the beam” approach. Separate hutches, away from beam lines, that can be used for staging were recommended. The European concept of “superusers” (external and internal) that are funded to develop capabilities that can then be shared by other researchers was introduced. This could include software/modeling as well as complex experimental modules, designed for general use (i.e. user friendly but adaptable).

B. Common Scientific Needs

Pressing Technical Problems: Several specific materials problems that are considered to be vital to technological challenges were brought up during the workshop:

- Develop an understanding of microstructure variability and the relationship of that variability to material failure such as crack initiation in fatigue and corrosion pitting. This requires a multiscale experimental/modeling approach.
- There is a need for a large-scale facility dedicated to environmental/corrosion science. Hydrogen in materials is a particularly ubiquitous phenomenon that affects many different technological problems. The details of where the hydrogen resides in the materials microstructure as a function of time and environment and the mechanisms of hydrogen induced material degradation are of vital interest to the community. This will require spatial resolution from μm to the atomic regime and temporal resolution down to the μs level.
- Materials processing provides many opportunities for the development of new, novel materials. Models might tell us what optimum structure is, but how do we develop these processes? For example, many structural material applications rely upon casting as the processing route because it is relatively quick, cheap and efficient. Most codes today only predict the thermal history of a casting, and then use either inference or empirical tools to predict microstructure in a general

sense. In order to become more predictive with our casting modeling codes, we need a better understanding of the microstructural processes occurring during solidification, e.g. nucleation and growth phenomena, chemical partitioning, grain orientation, and phase changes after solidification. For most applications this would need to be done at the micron scale and in the time scale of seconds.

Integrated Computational Materials Engineering (ICME): Modeling is integral to design and optimization in the development of advanced materials. Therefore a strong modeling component (software and hardware) is vital to the success of a facility like MaRIE. The link between modeling and experiment must be made throughout the material lifecycle: from manufacturing through performance to final retirement, with covalidation between experiments and models. From the industry perspective, cost needs to be an integral part of the modeling and materials design framework. Note that cost is not part of the traditional materials tetrahedron and may need to be included. This concept has been considered in detail by the National Materials Advisory Board of the National Research Council of the National Academies in their report: “Integrated Computation Materials Engineering (ICME)”¹. ICME is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation. In essence this is a design framework that integrates materials processing, microstructural, property, and performance models. Optimization via ICME reduces development time and costs and increases the confidence in fielding a new design.

Broad range of environments for in situ experiments: In situ experiments are particularly useful in understanding mechanisms in materials. There is a need to perform experiments under a broad range of environments, including stress, stress/strain rate, pressure, chemical environments, temperature, temperature rates/gradients, radiation, etc – and combinations of these. Defining and reproducing environments are both often difficult and will require multiple environmental factors imposed simultaneously on the specimen during the experiment. A flexible, modular design for experimental apparatus is particularly important to allow a wide range of environments to be explored.

Multiscale capability: Many materials problems require characterization of the sample on different length scales with varying resolution, even in the same experiment. Fatigue studies are a good example. Because of the stochastic nature of fatigue failure, the important life-limiting microstructural feature is not necessarily identified by monitoring a representative volume element (RVE), but the weakest volume element (WVE). A general survey of the sample, covering mm³ or greater volumes with relatively low spatial resolution is required initially to identify the initiation site (i.e. WVE) and its relationship to the overall microstructure, followed by more detailed analysis of this element during subsequent crack growth. This requires the ability to analyze data in real time to identify pertinent features and focus in on these features during the remainder of the experiment. Many other

¹ NAE ICME Report, 2008

examples of the need for this capability can be identified. This capability is the experimental complement to multiscale modeling. One suggestion was to combine multiple characterization tools and materials processing into a single connected instrument so that a material could be processed, exchanged in controlled environment to the characterization wing, transferred back to processing, and then transferred to further characterization of structure or properties.

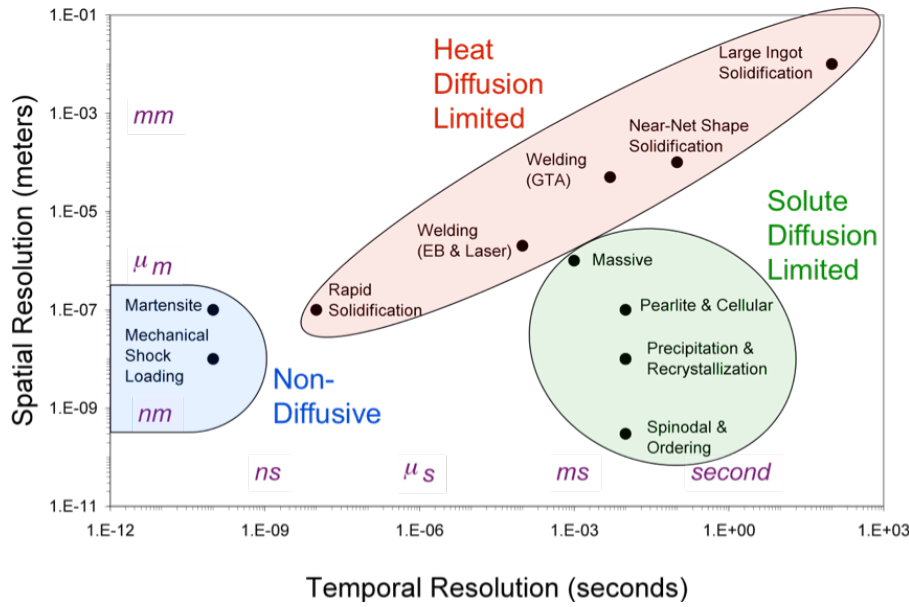


Figure 6. Resolution requirements for various phase transformation (R.E. Hackenberg, LANL)

Wide range of spatial and temporal resolution: The required spatial and temporal resolution is variable depending on the experiment and there are generally trade-offs between the two as well as the nature of the signal being collected. As stated above, different levels of resolution may be required within a single experiment. Temporal and spatial resolution are not as important for most structural materials as they are for functional materials, in which the operative mechanisms occur at atomic level in time intervals measured in picoseconds. Neither is temporal resolution as important here as it is for shock experiments (considered as separate issue for the sake of this report, since a separate workshop was conducted on this subject). However, the need for high spatial and temporal resolution is certainly present, particularly in cases where more detailed information is to be collected. For many of the structural materials applications of interest we would like timescales on the order of msec to sec. There are some applications that also require time resolution down to ns or μs for investigations of nucleation events, e.g. twin or martensite nucleation. The various regimes of temporal and spatial resolution required for a variety of phase transformation studies are summarized in Figure 6.

Multiple probes/detectors for simultaneous recording of disparate data: Once an experimental apparatus has been developed to produce a specific environment for in situ testing, the more information that can be collected during the experiment, the better the chance of obtaining a true understanding of the mechanisms being investigated. This requires multiple probes and detectors that can simultaneously gather data during the experiment. One example cited was the VULCAN diffractometer at the ORNL SNS facility, which combines small angle (SANS) and high angle detectors in the same instrument. One speaker stated that the ideal probe would have the “penetration of neutrons, detection speed of x-rays, and resolution of electrons”. Obviously a single probe cannot achieve this, but strides toward this ideal can be achieved using multiple probes, as well as multiple detectors to gather different aspects of the signal.

New detector technology optimized for Materials Science: Many talks focused on the need for improved detector technology for neutrons and X-rays: increased sensitivity, spherical shapes, semi-transparent, etc. Most beam users today rely on commercial technology developed by the medical imaging industry. With current technology, it may take several days to collect the multiple data sets (e.g. as a function of time in the environment or strain) for a single experiment. Advanced detector development can address this issue and represents a potential opportunity for MaRIE to help the overall scientific community. This would be relatively inexpensive compared to the development and construction of large beam lines.

3D analysis: Advanced n-D microstructural characterization techniques and the tools to analyze the enormous data sets are needed (n is 3D for spatial, plus time, grain orientation, strain, chemical signature, etc). Several examples were presented in which 2D characterization provided a false or incomplete understanding of the microstructure. The need for 3D analysis increases the time necessary for data collection as well as the amount of data collected. Current experimental capabilities (serial sectioning and EBSD analysis) require approximately 2 weeks to setup and collect grain orientation data with 1 μ m resolution and analyzed volume of 200 x 500 by 1000 μ m.

Data management and analysis: Data sets from some of the experiments referred to above are currently in the 3-10 Tb range and data analysis can take months to years. The increasingly large and complex (e.g. n-D) data sets that will arise from the experiments anticipated in the future demand a much more sophisticated approach to data management and analysis. Customer support in acquiring, storing, and processing the huge amount of information generated is vital for the user. In the words of one participant, a goal of MaRIE should be to “go from heroic to routine effort for analyzing the data collected”. There should be a parallel funding program to help with method development and data reduction. The goal should be to develop standardized data reduction and visualization algorithms, particularly for large 3D data sets, that are automated and user friendly (e.g. an interactive “gaming” interface).

Data archiving and sharing: Open sharing of data and analysis software is vital to the future development of new and novel materials. The need for curated, shared

databases, with standardized formats, was strongly emphasized. Several participants pointed to the medical and biological community as a model for the development and implementation of this concept. For example NIH requires that models and data developed using their funding be available to all who are funded by NIH.

C. User Facility Considerations

Flexible/modular design: One of the limiting factors at many large user facilities is the time that it takes to assemble the experimental apparatus on site. The more assembly that can be achieved before installation at the beam line site, the more efficient the facility becomes. A flexible design at the beam line that allows for modular experimental apparatus design, as well as staging areas for assembly, will greatly enhance the productivity of the user. Remote facility training will also allow users to take better advantage of their time on site.

Shared experimental tools: Once an apparatus has been built for a particular purpose, the ability for other users to take advantage of this equipment enhances its utility. The concept of the “Superuser” from European facilities was introduced. This class of user can be internal or external. He/she has more extensive access to the facility as well as development funds. In return, developments by this user must be available to others for their experiments.

User support: Customer support in setting up experiments, as well as acquiring, storing, and processing the huge amount of information generated is vital for the user. Coordinating communication/collaboration between experts in different fields is also necessary, as no individual has enough resources to develop these complex experiments alone.

Educational component: There is a need to develop the right kind of students and staff for a multi-disciplinary facility like MaRIE. Students have to be trained to work as a team and understand multiple disciplines as opposed to be narrowly focused on their specific research area. A summer school model similar to Lujan’s would also be appropriate.

Hazardous/difficult materials: The need for the ability to handle a wide variety of hazardous/difficult materials was emphasized. Given the mission of LANL, the ability to deal with radioactive materials and store them for future analysis after experiment is essential.

Ancillary facilities: A complete and up to date characterization facility for post mortem analysis is needed. This facility should have the ability bring to bear a combination of complimentary techniques for analyzing the specimen, e.g. TEM, SEM with focused ion beam (FIB) capability, and 3-D atom probe (LEAP). The ability to perform in situ experiments at this facility, such as dynamic TEM (DTEM) is also essential for any modern materials facility, as well a 3-D characterization (e.g. TEM tomography). On-site facilities as common such as machine shops are also recommended.

Computational capability: Modeling is also a critical component of any modern materials facility. This aspect has been discussed in previous sections, but is reiterated here. Advanced computational capabilities are a vital component to the integrated experimental/modeling approach.

D. MaRIE Specific Technical Recommendations

- An integrated modeling/experimental approach is vital to the future of materials development. The approach for MaRIE in this area should be consistent with ICME.
- Multiple in situ extreme environments are needed to simulate real life conditions as closely as possible and investigate complex mechanisms of materials degradation and failure. This will require a flexible facility that can accommodate complex experimental apparatus.
- Major breakthroughs in the understanding of fundamental materials phenomena will require simultaneously active multiple probes and detectors to fully characterize the specimen during in situ experiments.
- Coordinated multiscale modeling and experiments are critical to success. The latter will require multiple probes with a range of spatial and temporal resolution and real time analysis of data in order to zero in on “hot spots” in the microstructure for more detailed analysis.
- In addition to the advanced probes proposed for MaRIE, advanced detector development could have significant impact on the community at relatively low cost.
- Advanced n-D microstructural characterization techniques and the tools to analyze the enormous data sets are needed. (n is 3D for spatial, plus time, grain orientation, strain, chemical signature, etc).
- There is a need for a large-scale facility dedicated to environmental/corrosion science. MaRIE could fulfill this need.
- There is a need for a facility that can routinely handle radioactive/hazardous material, with the ability to store samples for further analysis. MaRIE could fulfill this need.
- There is a need for a large-scale facility for in situ characterization of materials during processing (e.g. casting, thermomechanical processing, welding, etc.). MaRIE could fulfill this need.
- State-of-the-art characterization and modeling tools are needed in addition to the “beamline tool” for a more enhanced experience for visiting users. Example: having SEM, TEM, FIB, atom probe, spectroscopy available to further characterize the sample ex situ, with transfer capability between in situ experimental site and ancillary capabilities.

- MaRIE should have a strong educational component to develop personnel for interdisciplinary teams needed for the future success of this type of facility.
- Shared experimental tools, data, and models would strongly enhance the impact of a user facility. A NIH model could be implemented. NIH requires that models and data be available to all who are funded by NIH. “Superusers” with enhanced funding/access would have a greater opportunity/responsibility for developing sharable tools.
- Customer support in setting up experiments, and acquiring, storing, and processing huge amounts of information is vital for the user. General software and hardware should be maintained by the facility, with personnel allocated to this function.
- Effective data archiving and open dissemination is central to the future of collaborative materials research. This must be developed upfront at a high level, not in an ad hoc manner by individual researcher/groups.
- The mission of MaRIE should focus on only 2-3 major materials challenges and address them comprehensively and holistically. MaRIE would develop personnel, tools and integrated models that solve complex problems and lead to new materials solutions.

“Structural Materials Under Extreme Conditions” MaRIE Workshop

**Materials Science Laboratory (MSL)
July 29 – July 31, 2009**

Wednesday, July 29th

7:15 – 8:20 Badging, Badge Office, TA-3, Bldg. 0261 Sheila Girard

AM Session: Materials Needs - Specific Applications – Chair: Dave Teter

8:30 – 8:40 Welcome/Announcements Dave Teter
LANL

8:40 – 9:10 MaRIE Overview John Sarrao
LANL

9:10 – 9:40 “Integrated Computational Materials Engineering:
A new and essential capability for surviving
extreme environments in the automotive industry” John Allison
Ford

9:40 – 9:50 Break

9:50 – 10:20 “Structural Materials Challenges in
Nuclear Energy Systems” Steve Zinkle
ORNL

10:20 – 10:50 “Aerospace Materials” Jim Williams
Ohio State U

10:50 – 11:20 “Materials Challenges in Oil and Gas
Industry” Greg Kusinski
Jim Skogsberg
Chevron

11:20 – 12:00 Discussion

12:00 – 1:30 Lunch (on your own)

PM Session: Materials Modeling – Chair: Carlos Tome

1:30 – 1:40	Session Introductions/Announcements	Carlos Tome LANL
1:40 – 2:15	“Modeling and Experimental Characterization of Local Features (stress, strain, microstructure)”	Carlos Tome LANL
2:15 – 2:50	“Interrogating Grain Scale Deformation within a Polycrystalline Alloy using New Micromechanical Testing Techniques and Crystal-Based Elastic Plastic Material Models”	Matthew Miller Paul Dawson Cornell U
2:50 – 3:05	Break	
3:05 – 3:40	“Multiscale Modeling of Deformation in Metals Under Extreme Conditions”	Hussein Zbib U Washington
3:40 – 4:15	“Phase Field Modeling of Coupled Displacive-Diffusional Processes”	Yunzhi Wang Ohio State U
4:15 – 5:15	Discussion	
5:15	Adjourn	
6:30	Informal Dinner	

Thursday, July 30th

AM Session: Materials Processing – Chair: Deniece Korzekwa

8:15 – 8:30	Session Introduction/Announcements	Deniece Korzekwa LANL
8:30 – 9:05	“Solidification Modeling and Experiments - What we think we know and what we need.”	Deniece Korzekwa LANL
9:05 – 9:40	“Role of Joining Science in Developing Hybrid Structural Materials”	Suresh Babu Ohio State U



9:40 – 9:55	Break	
9:55 – 10:30	“Radiation Effects on Metal/Oxide Interfaces”	Darryl Butt Boise State U
10:30 – 11:05	“Exploiting the Power of Powder Synthesis Reactions for Advanced Structural Materials”	Iver Anderson Ames Lab
11:05 – 12:00	Discussion	
12:00 – 1:30	Lunch (on your own)	
<i>PM Session: Characterization – Chair: Bob Field</i>		
1:30 – 1:40	Session Introduction/Announcements	Bob Field LANL
1:40 – 2:10	“In Situ Neutron Diffraction Techniques”	Sven Vogel LANL
2:10 – 2:40	“Characterization of Phase Transformations in Structural Materials Under Extreme Conditions”	Mike Kaufman Colo. Sch. Of Mines
2:40 – 3:10	“3D Microstructural Characterization and Analysis”	Andy Geltmacher Naval Res. Lab.
3:10 – 3:25	Break	
3:25 – 3:55	“High Energy X-ray Diffraction Microscopy: Access to Volumetric Microstructure Responses”	Robert Suter Carnegie-Mellon U
3:55 – 4:25	“In-situ 3D X-ray Techniques”	Erik Lauridsen RISO
4:25 – 5:30	Discussion	
5:30	Adjourn	

Friday, July 31st

AM Session: Specific Properties/Materials Interactions – Chair: Jim Foley

8:15 – 8:30	Session Introduction/Announcements	Jim Foley LANL
8:30 – 9:05	“Scientific Challenges Associated with Materials Degradation by Corrosion: Some Needs for Prognosis and Corrosion-Informed ICME”	John Scully U Virginia
9:05 – 9:40	“Hydrogen Embrittlement – Current Status and Future Directions”	Ian Robertson U Illinois
9:40 – 9:55	Break	
9:55 – 10:30	“Understanding the Role of Microstructure Variability on Fatigue Behavior”	Wayne Jones U Michigan
10:30 – 11:05	“High Temperature Materials: What Next?”	Tresa Pollock U Michigan
11:05 – 12:00	Discussion	
Noon	Adjournment	
PM:	Meeting of Organizers and Session Chairs	

Workshop Participants

Workshop Chairman: Bob Field, MST-6

Internal Organizers:

Dave Teter, MST-6
Carlos Tomé, MST-8
Deniece Korzekwa, MST-16
Jim Foley, MST-6

External Executive Committee:

Tresa Pollock (University of Michigan)
Ian Robertson (University of Illinois)
Darryl Butt (Boise State University)
Jim Williams (The Ohio State University)

Speakers:

John Allison (Ford Motor Company)
Steve Zinkle (Oak Ridge National Laboratory)
Jim Williams (The Ohio State University)
Greg Kusinski and Jim Skogsberg (Chevron)
Carlos Tome (Los Alamos National Laboratory)
Matthew Miller (Cornell University)
Hussein Zbib (University of Washington)
Yunzhi Wang (The Ohio State University)
Deniece Korzekwa (Los Alamos National Laboratory)
Suresh Babu (The Ohio State University)
Darryl Butt (Boise State University)
Iver Anderson (Ames Laboratory)
Sven Vogel (Los Alamos National Laboratory)
Mike Kaufman (Colorado School of Mines)
Andy Geltmacher (Naval Research Laboratory)
Robert Suter (Carnegie-Mellon University)
Erick Lauridsen (RISO, Denmark)
John R. Scully (University of Virginia)
Ian M. Robertson (University of Illinois)
J. Wayne Jones (University of Michigan)
Tresa Pollock (University of Michigan)

Other Attendees:

Addessio, Frank	T-3	Hosemann, Peter	MST-8
Alexander, David	MST-6	Knapp, Cameron	MST-6
Bai, Xian-Ming	MST-8	Korzekwa, David	MST-6
Barnes, Chris	P-DO	Lookman, Turab	T-4
Bingert, John	MST-8	Maloy, Stuart	MST-8
Blake, Nolen	MST-6	McCluskey, Mark	MPA-MC
Bourke, Mark	MST-8	Nastasi, Mike	MPA-CINT
Budiman, Arief	MPA-CINT	Necker, Carl	MST-6
Cerreta, Ellen	MST-8	Orler, Bruce	MST-7
Chan, Shao-Ping	T-1	Pena, Maria	MST-6
Cieslak, Wendy	MST-DO	Sanders, Billy	UC-Davis
Clark, Blythe	SNL	Shlachter, Jack	ADEPS
Clarke, Amy	MST-6	Sintay, Stephen	CCS-2
Clarke, Kester	MST-6	Stan, Marius	CCS-2
Da, B. C.	SNL	Thoma, Dan	MDI
Devaurs, Micheline	SPO-SC	Valone, Steve	MST-8
Devlin, David	MST-7	Van den Bosch, Joris	MST-8
Di, Zengfeng	MPA-CINT	Van, Igor	MST-8
Dunn, Paul	MST-DO	Way, Zhiqiang	T-3
Farrow, Adam	MST-16	Wei, Qiangmin	MPA-CINT
Gibbs, John	MST-6	Xu, Wei	MPA-CINT
Hatter, Ghalid	SNL	Zocco, Adam	MST-6
Hill, Mary Ann	MST-6		
Horfer, Khalid	T-8		